

New inroads in an old subject: plasticity, from around the atomic to the macroscopic scale

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Abstract

Nonsingular, stressed, dislocation (wall) profiles are shown to be 1-d equilibria of a non-equilibrium theory of Field Dislocation Mechanics (FDM). It is also shown that such equilibrium profiles corresponding to a given level of load cannot generally serve as a traveling wave profile of the governing equation for other values of nearby constant load; however, one case of soft loading with a special form of the dislocation velocity law is demonstrated to have no ‘Peierls barrier’ in this sense. The analysis is facilitated by the formulation of a 1-d, scalar, time-dependent, Hamilton-Jacobi equation as an exact special case of the full 3-d FDM theory accounting for non-convex elastic energy, small, Nye-tensor dependent core energy, and possibly an energy contribution based on incompatible slip. Relevant nonlinear stability questions are formulated in a non-equilibrium setting. Elementary averaging ideas show a singular perturbation structure in the evolution of the (unsymmetric) macroscopic plastic distortion, thus pointing to the possibility of predicting generally rate-insensitive slow response constrained to a tensorial ‘yield’ surface, while allowing fast excursions off it, even though only simple kinetic assumptions are employed in the microscopic FDM theory. The emergent small viscosity on averaging that serves as the small parameter for the perturbation structure is a robust, almost-geometric consequence of large gradients of slip in the dislocation core and the presence of a large number of dislocations in the averaging volume. In the simplest approximation, the macroscopic yield criterion displays anisotropy based on the microscopic dislocation line and Burgers vector distribution, a dependence on the Laplacian of the incompatible slip tensor and a nonlocal term related to a Stokes-Helmholtz-curl projection of an ‘internal stress’ derived from the incompatible slip energy.

1. Introduction

We are concerned here with the development of an idealized mathematical description of nominally crystalline solids containing dislocations as the only defects. The interest is in behavior at the time scale of \sim microseconds or more and therefore in theory that can be routinely used for attempting to understand such behavior. It is our belief that an appropriate, nonlocal field/continuum description that involves fields that are smooth over a length scale of interatomic length and larger can be adequate for such a purpose. Kinetic energy of atomic and subatomic vibrations below this length scale, and time averaged over periods of microseconds, is characterized as dissipation within such a framework. Thus, in concept, we exchange the atoms and their (sub)femtosecond vibration periods in Molecular Dynamics with the dissipative evolution of a mathematical dislocation density field (capable of representing ‘individual’ dislocations) within a nominally elastic continuum characterized eventually by Cauchy-Born crystal elasticity (Milstein, 1982; Ortiz and Phillips, 1999). The stored energy of the body is augmented with some additional contributions to represent nonlocal energy content that cannot be ascribed to local elastic response, but hopefully with enough physical meaning so as to be capable of unambiguous definition from quantum/atomistic studies. Our main goal in pursuing this direction of work is really the prediction of the *dynamics* of mesoscale microstructure and its effect on macroscopic properties; since temporal coarse-graining of MD remains elusive and a rational discrete-to-continuum transition in the 3-d, time-dependent setting even more so in the

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presence of large numbers of defects, we believe that it is important to understand exactly what can and cannot be achieved by an atomic scale field theory grounded in sound kinematics, conservation statements, and the possibility of fitting necessary physics from subatomic scales, since such a framework has the potential of being an effective unified tool for achieving the desired scale transitions. We provide a very first demonstration of this overall approach in the paper, and, of course, much remains to be done.

We pursue work here in the geometrically linear setting for two reasons. First, the continuum mechanics and physical ideas involved are sufficiently non-standard to warrant leaving aside the complications due to geometric nonlinearity for the moment. Second, for a part of the present model, the extension to finite deformations exists in Acharya (2004), and extending that earlier work to account for the new developments, while technically intricate from the continuum mechanics perspective, would be conceptually straightforward.

An interesting conceptual issue comes up in this work related to the definition of the condition for the onset of motion of a single dislocation, especially when compared to the treatment of the same question as initiated in Peierls (1940) based on the static, classical, elastic theory of dislocations. Due to the translational invariance of the sum of the linear elastic and the interplanar energy of an infinite body in that analysis, the dislocation core could be situated anywhere on the slip plane with the same energy cost. This prompted Peierls to conclude that, within that theory, there could not be a threshold stress to initiate rigid motion of a dislocation to move it from one location to another. A stronger result is shown by Movchan et al. (1998) in that an equilibrium solution to the problem with a non-zero, but small, applied stress does not exist. Peierls's (1940) conclusion and preliminary work prompted the accounting of lattice discreteness in the theory of the Peierls stress (Nabarro, 1947) followed by a rich literature (e.g. Picu, 2002), whereby invariance of the energy with respect to all continuous spatial translations of its argument fields is exchanged for discrete invariance respecting the symmetry of the lattice (e.g. Lu et al., 2000).

The model presented in this paper is translationally invariant. It is also dynamic, even in the absence of inertia. In the context of the static approach to the Peierls stress problem, while the absence of an equilibrium configuration under small load is a compelling result, it is perhaps fair to say that this result by itself does not say anything about how the dislocation profile evolves under non-zero load – e.g. does instability lead to a complete collapse of the slip configuration, or a very severe distortion with no semblance to a slip profile representing a dislocation, or does it mean rigid translation of the equilibrium profile corresponding to no load? Or, very importantly, does the dislocation density profile evolve, but with indiscernible translation of the dislocation core up to a certain value of the load after which there is an almost rigid translation? What effect does rate of loading and temperature have on this experiment? It seems that a dynamical model, with a basis in mechanics (e.g. the discrete Peierls model of Movchan et al., 1998), is required for such a purpose. Thus, we pose the question of existence of a barrier to *rigid* translation as one of determining when dislocation-like equilibrium profiles under zero load may not serve as traveling wave profiles under load, realizing full well that the practically relevant criterion would be related to “almost rigid” translation, but defining the latter precisely is far more delicate than the former. In a simplified 1-d setting, we show that the answer varies with the choice of dislocation velocity law and loading mode (displacement or traction control), and clearly translational invariance is not the crux of the issue in this model. Of course, our general theory does not preclude the inclusion of discrete translational invariance in the model through physically appropriate modifications to the form of the energy density function, in the

spirit of the semi-discrete Peierls model (Lu et al., 2000) and/or through a restatement in the language of discrete calculus (e.g. Ariza and Ortiz, 2005).

This paper is organized as follows: in Section 2 we settle on some notational conventions. Section 3 describes the theoretical framework. In Section 4 a simple, but exact, model problem is developed and the general theory is applied to it. We obtain some special exact solutions for equilibria and a travelling wave, and formulate some questions of dynamical stability whose answers would be of direct physical interest. In Section 5 we consider preliminary implications of our atomic-scale model on meso and macroscopic response. In Section 6 we present some comparative observations on aspects of our model with time-dependent Ginzburg Landau models and level-set propagation.

2. Notation

A superposed dot on a symbol represents a material time derivative. The statement $a := b$ is meant to indicate that a is being defined to be equal to b . The summation convention is implied. We denote by $\mathbf{A}\mathbf{b}$ the action of the second-order (third-order, fourth-order) tensor \mathbf{A} on the vector (second-order tensor, second-order tensor) \mathbf{b} , producing a vector (vector, second-order tensor). $\mathbf{A} \cdot$ represents the inner product of two vectors, $\mathbf{A} :$ represents the trace inner product of two second-order tensors (in rectangular Cartesian components, $\mathbf{A} : \mathbf{B} = A_{ij}B_{ij}$) and matrices. The symbol \mathbf{AB} represents tensor multiplication of the second-order tensors \mathbf{A} and \mathbf{B} . The *curl* operation and the cross product of a second-order tensor and a vector are defined in analogy with the vectorial case and the divergence of a second-order tensor: for a second-order tensor \mathbf{A} , a vector \mathbf{v} , and a spatially constant vector field \mathbf{c} ,

$$\begin{aligned} (\mathbf{A} \times \mathbf{v})^T \mathbf{c} &= (\mathbf{A}^T \mathbf{c}) \times \mathbf{v} \quad \forall \mathbf{c} \\ (\text{div } \mathbf{A})^T \mathbf{c} &= \text{div}(\mathbf{A}^T \mathbf{c}) \quad \forall \mathbf{c} \\ (\text{curl } \mathbf{A})^T \mathbf{c} &= \text{curl}(\mathbf{A}^T \mathbf{c}) \quad \forall \mathbf{c}. \end{aligned} \tag{1}$$

In rectangular Cartesian components,

$$\begin{aligned} (\mathbf{A} \times \mathbf{v})_{im} &= e_{mjk} A_{ij} v_k \\ (\text{div } \mathbf{A})_i &= A_{ij,j} \\ (\text{curl } \mathbf{A})_{im} &= e_{mjk} A_{ik,j}, \end{aligned} \tag{2}$$

where e_{mjk} is a component of the *third-order alternating tensor* \mathbf{X} . The spatial derivative, for the component representation is with respect to rectangular Cartesian coordinates on the body. For all manipulations with components, we shall always use such rectangular Cartesian coordinates. The symbol *div* represents the divergence, *grad* the gradient, and *div grad* the Laplacian. We often have occasion to use the identity $\text{curl } \text{curl}(\cdot) = \text{grad } \text{div}(\cdot) - \text{div } \text{grad}(\cdot)$, often for an argument for which $\text{div}(\cdot) = 0$

3. Field Dislocation Mechanics

The theory utilizes a continuum description of defect density based on the incompatibility of elastic distortion. As such, it is potentially applicable to materials for which an elastic response is

defined (e.g. amorphous materials like metallic glasses); in this paper we associate the defect density field α with a continuously distributed dislocation density in crystalline materials with single dislocations viewed as non-singular, spatially localized structures in this continuously distributed density field. The utility of such a representation, even for the visualization of core structures from computer simulations, is demonstrated in Hartley and Mishin (2005)¹.

The elastic distortion of the lattice is represented by the (generally nonsymmetric) tensor \mathbf{U}^e . Due to lattice incompatibility, the elastic distortion is not generally a gradient of a vector field and we write its incompatibility field as

$$\text{curl} \mathbf{U}^e =: \alpha. \quad (3)$$

Since we insist that the total observable displacement gradient field (from an arbitrarily chosen reference configuration, say B) be the sum of the plastic distortion, \mathbf{U}^p (with respect to that reference), and the elastic distortion, the plastic distortion is also not in general a gradient;

$$\text{grad} \mathbf{u} = \mathbf{U}^e + \mathbf{U}^p \Rightarrow \text{curl} \mathbf{U}^e = -\text{curl} \mathbf{U}^p. \quad (4)$$

It is written as a sum of a gradient and an incompatible part (that cannot be expressed as a gradient)

$$\mathbf{U}^p = \text{grad} \mathbf{z} - \chi. \quad (5)$$

The incompatible part results from the distribution α through the fundamental geometrical equation of incompatibility

$$\text{curl} \mathbf{U}^p = -\alpha \Rightarrow \text{curl} \chi = \alpha \quad (6)$$

with the side condition

$$\begin{aligned} \text{div} \chi &= \mathbf{0} \quad \text{on } B \\ \chi \mathbf{n} &= \mathbf{0} \quad \text{on the boundary } \partial B \text{ with unit normal } \mathbf{n} \end{aligned} \quad (7)$$

to ensure that when $\alpha \equiv \mathbf{0}$ the incompatible part χ vanishes identically on the body. Thus, (5) may be interpreted as the Stokes-Helmholtz decomposition of \mathbf{U}^p into a gradient field and a curl field (see (22) below). The compatible part $\text{grad} \mathbf{z}$ depends upon the history of plastic straining and accumulates the compatible increments of the plastic strain produced by the motion of the dislocation density through the equation

$$\text{div} \text{grad} \dot{\mathbf{z}} = \text{div}(\alpha \times \mathbf{V}). \quad (8)$$

In this model of dislocation mechanics, the total displacement field, \mathbf{u} , does not represent the actual physical motion of atoms involving topological changes but only a consistent shape change and hence is not required to be discontinuous. However, the stress produced by these topological changes in the lattice is adequately reflected in the theory through the utilization of incompatible elastic/plastic distortions. As usual in continuum plasticity, the stress is a function of the elastic distortion (in the linear elastic case given by $\mathbf{T} = \mathbf{C}\mathbf{U}^e$). While not necessary in the context of the general theory, in this paper we focus on defect dynamics in the presence of static force balance characterized by

$$\text{div} \mathbf{T} = \mathbf{0}. \quad (9)$$

The definition (3) locally renders α as a density of lines carrying a vectorial attribute (the Burgers vector), and it is natural to associate a velocity field that moves these line segments in

¹ The paper contains some unfortunate typographical errors that cloud the exposition of the method. Also, the link that the authors wish to demonstrate with Bilby's lattice correspondence functions could not be followed by this author, but thankfully that link is not a relevant part of the essential construction of the paper.

the body. This idea can be made geometrically rigorous and results in the fundamental conservation law (due to Mura (1963) who attributes it to Kröner):

$$\dot{\boldsymbol{\alpha}} = -\text{curl}(\boldsymbol{\alpha} \times \mathbf{V}), \quad (10)$$

where the field \mathbf{V} at any spatio-temporal location represents the velocity of the infinitesimal dislocation segment at that location. Gathering all equations, the complete theory reads as

$$\left. \begin{aligned} \text{curl } \boldsymbol{\chi} &= \boldsymbol{\alpha} \\ \text{div } \boldsymbol{\chi} &= \mathbf{0} \\ \text{div}(\text{grad } \dot{\mathbf{z}}) &= \text{div}(\boldsymbol{\alpha} \times \mathbf{V}) \\ \mathbf{U}^e &:= \text{grad}(\mathbf{u} - \mathbf{z}) + \boldsymbol{\chi} \\ \text{div}[\mathbf{T}(\mathbf{U}^e)] &= \mathbf{0} \\ \dot{\boldsymbol{\alpha}} &= -\text{curl}(\boldsymbol{\alpha} \times \mathbf{V}) \end{aligned} \right\} \text{ on } B. \quad (11)$$

As for boundary conditions,

$$\left. \begin{aligned} \boldsymbol{\chi} \mathbf{n} &= \mathbf{0} \\ (\text{grad } \dot{\mathbf{z}} - \boldsymbol{\alpha} \times \mathbf{V}) \mathbf{n} &= \mathbf{0} \end{aligned} \right\} \text{ on } \partial B \quad (12)$$

are imposed along with standard conditions on displacement and/or traction. For the dislocation density field, analysis from the linear partial differential equation point of view indicates (Acharya, 2003) that it suffices to prescribe $\boldsymbol{\alpha}(\mathbf{V} \cdot \mathbf{n})$ on inflow parts of the boundary, but we believe that the nonlinear problem admits other physically motivated possibilities (Acharya and Roy, 2006).

3.1 Dissipation

In (11)-(12) the functions \mathbf{T} and \mathbf{V} need to be constitutively specified. We seek guidance in doing so by following a global analog of parts of a procedure initiated by Coleman and Noll (1963) and Coleman and Gurtin (1967) for local constitutive equations. A specific free energy density function is introduced as follows:

$$\begin{aligned} \psi &= \hat{\psi}(\mathbf{U}_{sym}^e) + s(|\boldsymbol{\alpha}|l)G(\boldsymbol{\chi}) + \frac{\varepsilon}{2} \boldsymbol{\alpha} : \boldsymbol{\alpha}, \\ s(x) &:= x^{\frac{1}{m}}, \quad x \geq 0, \quad m \gg 1, \end{aligned} \quad (13)$$

where l is a typical interatomic distance, e.g. Burgers vector magnitude, of the crystal.

The first term contains the contribution to the stored energy due to deformation of the lattice due to the application of loads and the presence of dislocations – since we are interested in nonlinear crystal elasticity respecting the symmetries of a lattice, this contribution is in inherently nonlinear due to lattice periodicity.

The second term reflects a local dependence on incompatible slip in dislocated regions. To the extent that any energy is physically understood, it seems reasonable to demand that it be defined purely in terms of the observed state. It is for this reason that only the incompatible slip, completely identifiable from the observable, instantaneous dislocation density field, occurs as an argument of the stored energy and not the whole of the plastic distortion \mathbf{U}^p as the latter contains the compatible part, $\text{grad } \mathbf{z}$, whose knowledge requires knowledge of the history of

dislocation motion (11)₃. The function s ensures that the energy due to incompatible slip is taken into account only in regions where the lattice has a ‘fault’, as reckoned by the dislocation density. Thus, even though a volumetric density, if dislocated regions are localized around planes, this energy contribution is also localized similarly.

The third term, with $\varepsilon = O(\mu l^2)$ where μ is a typical elastic modulus, represents the fact that the dislocation density in the body cannot be greater in order of magnitude than roughly $\sim 1/l$. The physical justification for the statement is that a gradient in elastic distortion can be reliably measured over a minimal distance of l in a crystal. Thus, ε is to be thought of as a small parameter. Alternatively, the term may also be thought of as an energy contribution in the material that arises in the presence of high gradients of incompatible lattice distortion.

Taken together, the last two terms in (13) are meant to represent the fact that a solely *local* elastic energy response, even though nonconvex, may not suffice to represent the energy content of a material element at the atomic scale, if it happens to contain incompatible gradients of slip. Clearly, we are thinking of the body as a continuum containing material points even in the regions between successive atomic planes and that such points are capable of transmitting forces between themselves. We hope that the dominant qualitative characteristics of actual nonlinear and nonlocal energy of a defected lattice can be represented by the postulated general energy in (13) but, of course, proving the correspondence in a physically rigorous manner is not obvious, and less so mathematically.

We define the mechanical dissipation in the body as the difference of the power of the applied forces and rate of change of the stored energy, i.e.

$$D = \int_{\partial B} (\mathbf{T}\mathbf{n}) \cdot \dot{\mathbf{u}} \, da - \int_B \dot{\psi} \, dv = \int_B \mathbf{T} : \text{grad } \dot{\mathbf{u}} \, dv - \int_B \dot{\psi} \, dv, \quad (14)$$

where we have ignored inertia represented in the displacement field, but including it poses no special problems.

Our modest goal now is to make choices for \mathbf{V} and \mathbf{T} that ensure $D \geq 0$. On assuming

$$\mathbf{T} = \frac{\partial \psi}{\partial \mathbf{U}_{\text{sym}}^e} \quad (15)$$

consistent with elasticity, the dissipation may be written as

$$D = \int_B \mathbf{T} : \dot{\mathbf{U}}^p \, dv - \int_B \varepsilon \boldsymbol{\alpha} : \dot{\boldsymbol{\alpha}} \, dv - \int_B s(|\boldsymbol{\alpha}|l) \frac{\partial G}{\partial \boldsymbol{\chi}} : \dot{\boldsymbol{\chi}} \, dv - \int_B G s'(|\boldsymbol{\alpha}|l) l |\dot{\boldsymbol{\alpha}}| \, dv. \quad (16)$$

\mathbf{V} needs to appear in (16) in order to identify its driving force. To this end, we first show that the structure of the equations (11)-(12) imply $\dot{\mathbf{U}}^p = \boldsymbol{\alpha} \times \mathbf{V}$. Equations (5), (11)_{1,3,6} imply

$$\begin{aligned} \text{curl } \dot{\mathbf{U}}^p &= \text{curl}(\boldsymbol{\alpha} \times \mathbf{V}) \\ \text{div } \dot{\mathbf{U}}^p &= \text{div}(\boldsymbol{\alpha} \times \mathbf{V}). \end{aligned} \quad (17)$$

(17)₁ implies the existence of a vector field², say \mathbf{a} , such that $\dot{\mathbf{U}}^p - \boldsymbol{\alpha} \times \mathbf{V} = \text{grad } \mathbf{a}$, and then

(17)₂ implies that \mathbf{a} satisfies Laplace’s equation

$$\text{div grad } \mathbf{a} = \mathbf{0} \text{ on } B. \quad (18)$$

Now, on the boundary ∂B , $\dot{\mathbf{U}}^p \mathbf{n} = -\dot{\boldsymbol{\chi}} \mathbf{n} + \text{grad } \dot{\boldsymbol{\chi}} \mathbf{n} = (\boldsymbol{\alpha} \times \mathbf{V}) \mathbf{n}$ from (5), (12)_{1,2}; therefore,

² Assuming the required degree of triviality in the topology of the body.

$$(\text{grad } \mathbf{a})\mathbf{n} = \mathbf{0} \quad \text{on } \partial B. \quad (19)$$

Consequently, (18) and (19) along with the uniqueness of solutions Laplace's equation with Neumann boundary conditions (up to constant fields) implies

$$\text{grad } \mathbf{a} = \mathbf{0} \Rightarrow \boxed{\dot{\mathbf{U}}^p = \boldsymbol{\alpha} \times \mathbf{V}}. \quad (20)$$

Hence, the dissipation may be written, utilizing (5), (11)₆ and (20) as

$$D = \int_B \mathbf{T} : (\boldsymbol{\alpha} \times \mathbf{V}) dv + \int_B \varepsilon \boldsymbol{\alpha} : \text{curl}(\boldsymbol{\alpha} \times \mathbf{V}) dv - \int_B \mathbf{R} : \dot{\boldsymbol{\chi}} dv \quad ; \quad \mathbf{R} := s(|\boldsymbol{\alpha}|l) \frac{\partial G}{\partial \boldsymbol{\chi}}. \quad (21)$$

In writing (21) we have essentially ignored the contribution from the last term in (16). For m large, s is essentially the constant function with value 1, except near zero. By carrying along the ignored contribution through to equation (27) below, it can be seen that ignoring this term from (21) onwards implies no loss in generality. In any case, this whole exercise is meant to motivate a constitutive assumption for \mathbf{V} , and ignoring the said term may just as well be considered as part of this assumption.

To manipulate the last term on the right-hand-side of (21), we utilize a Stokes-Helmholtz resolution of a square-integrable tensor field with square-integrable gradients due to Friedrichs (see, e.g., Jiang, 1998, Theorems 5.8, 5.2). The resolution states that given such a tensor field \mathbf{R} , there exists a unique (up to a constant) vector field \mathbf{g}_R and a unique tensor field \mathbf{W}_R satisfying

$$\begin{aligned} -\text{div grad } \mathbf{W}_R &= \text{curl } \mathbf{R} \quad ; \quad \text{div } \mathbf{W}_R = \mathbf{0} \quad \text{on } B \\ \mathbf{W}_R \times \mathbf{n} &= \mathbf{0} \quad \text{on } \partial B \\ \text{div grad } \mathbf{g}_R &= \text{div } \mathbf{R} \quad ; \quad (\text{grad } \mathbf{g}_R - \mathbf{R})\mathbf{n} = \mathbf{0} \quad \text{on } \partial B \quad \text{and} \\ \mathbf{R} &= \text{curl } \mathbf{W}_R + \text{grad } \mathbf{g}_R \quad \text{on } B. \end{aligned} \quad (22)$$

In keeping with the decomposition of the plastic distortion, we alternatively refer to $\text{curl } \mathbf{W}_R$ as

$$\boldsymbol{\chi}_R := \text{curl } \mathbf{W}_R. \quad (23)$$

Utilizing this decomposition, (11)_{2,6} and (12)₁,

$$\int_B \mathbf{R} : \dot{\boldsymbol{\chi}} dv = - \int_B \mathbf{W}_R : \text{curl}(\boldsymbol{\alpha} \times \mathbf{V}) dv. \quad (24)$$

Therefore,

$$\boxed{D = \int_B \left\{ \mathbf{X} \left(\mathbf{T} + [\varepsilon \text{curl } \boldsymbol{\alpha} + \text{curl } \mathbf{W}_R]^T \right) \boldsymbol{\alpha} \right\} \cdot \mathbf{V} dv - \varepsilon \int_{\partial B} \boldsymbol{\alpha} : [(\boldsymbol{\alpha} \times \mathbf{V}) \times \mathbf{n}] da}, \quad (25)$$

utilizing the fact that $\mathbf{W}_R : [(\boldsymbol{\alpha} \times \mathbf{V}) \times \mathbf{n}] = -(\boldsymbol{\alpha} \times \mathbf{V}) : (\mathbf{W}_R \times \mathbf{n}) = 0$ on ∂B due to (22).

We assume that the boundary term is dominated by the interior term, thus identifying the 'driving force' for the dislocation velocity field as

$$\mathbf{V} \rightarrow \mathbf{X} \left(\mathbf{T} + [\varepsilon \text{curl } \boldsymbol{\alpha} + \boldsymbol{\chi}_R]^T \right) \boldsymbol{\alpha}. \quad (26)$$

Here we consider simple kinetic assumptions of the form

³ In applying this decomposition to (5), (7) note that $\mathbf{W}_{U^p} \times \mathbf{n} = \mathbf{0}$ on ∂B implies that the line integral of \mathbf{W}_{U^p} on arbitrary closed curves on the boundary ∂B vanishes so that by Stokes theorem, $\text{curl } \mathbf{W}_{U^p} \mathbf{n} = -\boldsymbol{\chi} \mathbf{n} = \mathbf{0}$ on ∂B .

$$\mathbf{V} = \frac{\mathbf{X} \left(\mathbf{T} + [\varepsilon \text{curl } \boldsymbol{\alpha} + \boldsymbol{\chi}_R]^T \right) \boldsymbol{\alpha}}{\tilde{B}} \quad ; \quad \tilde{B} > 0 \quad (27)$$

$$\tilde{B} = \begin{cases} B \\ B^* |\boldsymbol{\alpha}| \end{cases} \quad \text{where } B, B^* \text{ are material constants,}$$

and the physical dimensions of \tilde{B} is that of $\text{stress} \times (\text{length})^{-1} \times (\text{velocity})^{-1}$. It is to be noted that a ‘classical’ dislocation is identified in this model as a region of linear dimension of l (the core) over which the incompatible slip varies continuously by an $O(1)$ amount; assumption (27) implies that in this model the dislocation velocity field actually varies significantly in this region.

With this constitutive assumption, the governing equation for $\boldsymbol{\alpha}$, a tensorial conservation law, is given by

$$\dot{\boldsymbol{\alpha}} = -\text{curl} \left(\boldsymbol{\alpha} \times \frac{\mathbf{X} \left(\mathbf{T} + [\varepsilon \text{curl } \boldsymbol{\alpha} + \boldsymbol{\chi}_R]^T \right) \boldsymbol{\alpha}}{\tilde{B}(|\boldsymbol{\alpha}|)} \right). \quad (28)$$

The corresponding governing equation for the plastic distortion is inferred from (20) as

$$\dot{\mathbf{U}}^p = \text{curl} \mathbf{U}^p \times \frac{\mathbf{X} \left(\mathbf{T} + [-\varepsilon \text{div grad } \boldsymbol{\chi} + \boldsymbol{\chi}_R]^T \right) \text{curl} \mathbf{U}^p}{\tilde{B}(|\text{curl} \mathbf{U}^p|)}. \quad (29)$$

Of course, *the jump conditions/continuity requirements for the plastic distortion cannot be inferred from (29) without knowledge of the form of the physical conservation law (28)*. Equation (29) is a ‘nonlocal’ (due to the term $\boldsymbol{\chi}_R$), nonlinear system of second-order PDE, with the flavor of a coupled system of first-order Hamilton-Jacobi equations involving wave-phenomena, singularly perturbed by a second-order term (Laplacian) but in a nonlinear manner.

4. Shearing of a bar

Consider a problem where only the

$$U_{12}^e \quad (30)$$

component of \mathbf{U}^e is non-vanishing and all fields vary only in the x_3 direction. So, x_3 is the axis of an infinite cylinder say of square cross section. Let x_1, x_2 be orthogonal directions in the cross section. Then the only non-vanishing components of the Nye tensor $\boldsymbol{\alpha}$ are

$$\varepsilon_{132} U_{12,3}^e = \alpha_{11} \quad \Rightarrow \quad \alpha_{11} = -U_{12,3}^e.$$

We assume that the only nonvanishing stress components are

$$T_{12} = T \left(\frac{1}{2} (U_{12}^e + U_{21}^e) \right) = T_{21}$$

which vary only in the x_3 direction and so equilibrium ($T_{ij,j} = 0$) is identically satisfied regardless of the x_3 variation of \mathbf{U}^e . Assume that required shear tractions can be mobilized on the lateral surfaces of the cylinder.

For simplicity, we now assume that $\text{curl} \mathbf{W}_R$ is symmetric and, like the stress, that $(\text{curl} \mathbf{W}_R)_{12}$ is the only nonvanishing component (up to symmetry).

Now,

$$\frac{\partial \boldsymbol{\alpha}}{\partial t} = -\text{curl}(\boldsymbol{\alpha} \times \mathbf{V})$$

where \mathbf{V} is given by (27). Consider the term

$$f_i := \varepsilon_{ijk} T_{jr} \alpha_{rk} \quad ; \quad \mathbf{f} = \mathbf{X} \mathbf{T} \boldsymbol{\alpha}.$$

The only non-vanishing components of $T_{jr} \alpha_{rk}$ is given by

$$T_{2r} \alpha_{r1} = T_{21} \alpha_{11} = T_{12} \alpha_{11}$$

so that the only non-vanishing component of \mathbf{f} is

$$f_3 = \varepsilon_{321} T_{21} \alpha_{11} = -T_{21} \alpha_{11}. \quad (31)$$

Now

$$\begin{aligned} (\boldsymbol{\alpha} \times \mathbf{f})_{ri} &= \varepsilon_{ijk} \alpha_{rj} f_k = \varepsilon_{ij3} \alpha_{rj} f_3 = \varepsilon_{i13} \alpha_{r1} f_3 + \varepsilon_{i23} \alpha_{r2} f_3 \\ (\boldsymbol{\alpha} \times \mathbf{f})_{r2} &= -\alpha_{r1} f_3 \\ (\boldsymbol{\alpha} \times \mathbf{f})_{r1} &= \alpha_{r2} f_3. \end{aligned} \quad (32)$$

So

$$[\text{curl}(\boldsymbol{\alpha} \times \mathbf{f})]_{ri} = \varepsilon_{isp} (\boldsymbol{\alpha} \times \mathbf{f})_{rp,s} = \varepsilon_{is1} (\boldsymbol{\alpha} \times \mathbf{f})_{r1,s} + \varepsilon_{is2} (\boldsymbol{\alpha} \times \mathbf{f})_{r2,s}.$$

Therefore the only non-vanishing component of $\text{curl}(\boldsymbol{\alpha} \times \mathbf{f})$ is

$$[\text{curl}(\boldsymbol{\alpha} \times \mathbf{f})]_{11} = \varepsilon_{132} (\boldsymbol{\alpha} \times \mathbf{f})_{12,3} = -(\boldsymbol{\alpha} \times \mathbf{f})_{12,3} = (\alpha_{11} f_3)_{,3}. \quad (33)$$

Of course, under the assumptions we have made, one can use similar arguments to deal with the term $\text{curl} \mathbf{W}_R$ in the expression for the dislocation velocity. The remaining term to deal with is $\mathbf{X}(\text{curl} \boldsymbol{\alpha})^T \boldsymbol{\alpha}$. Since α_{11} is the only non-zero component of the dislocation density, the only survivor in

$$(\text{curl} \boldsymbol{\alpha})_{ij} = e_{jmn} \alpha_{in,m}$$

is $(\text{curl} \boldsymbol{\alpha})_{12} = e_{j31} \alpha_{11,3} = \alpha_{11,3}$. Therefore, the only non-zero survivor in

$$\left(\mathbf{X}(\text{curl} \boldsymbol{\alpha})^T \boldsymbol{\alpha} \right)_s = e_{sjr} \left\{ (\text{curl} \boldsymbol{\alpha})^T \right\}_{ji} \alpha_{ir}$$

is

$$\left(\mathbf{X}(\text{curl} \boldsymbol{\alpha})^T \boldsymbol{\alpha} \right)_3 = e_{321} \left\{ (\text{curl} \boldsymbol{\alpha})^T \right\}_{21} \alpha_{11} = -\alpha_{11,3} \alpha_{11}. \quad (34)$$

Noting (31)-(34), it can now be deduced that the evolution equation for the only non-zero component of the dislocation density tensor is

$$\dot{\alpha}_{11} = - \left\{ \frac{1}{\tilde{B}(\alpha_{11})} \alpha_{11} \left[-\alpha_{11} (T_{12} + (\boldsymbol{\chi}_R)_{12} + \varepsilon \alpha_{11,3}) \right] \right\}_{,3}. \quad (35)$$

We now assume $u_{1,2}$ to be the only non-zero displacement gradient component which is only a function of x_3 and t . Along with (30), this implies that U_{12}^p is the only non-zero plastic distortion component and further that

$$\alpha_{11} = -e_{132} U_{12,3}^p = U_{12,3}^p. \quad (36)$$

Let us denote

$$\varphi(x, t) := U_{12}^P(x, t) \quad ; \quad x \equiv x_3 \quad (37)$$

Henceforth, a subscript x will denote partial differentiation w.r.t x , and similarly with t . Using (31), (32)₂, and (34), (29) now reduces to

$$\varphi_t = \frac{(\varphi_x)^2}{\tilde{B}(|\varphi_x|)} [T_{12} + \varepsilon \varphi_{xx} + \chi_{R12}], \quad (38)$$

using the fact that $-\text{div grad } \chi = \text{curl } \alpha$. The primary reason why the 1-d scalar version of the Laplacian in χ can be written in terms of the full plastic distortion (φ_{xx}) is that in this simplified problem $\text{div}(\alpha \times V) = 0$.

For the sake of simplifying analysis in a special case, we would like to have (38) solely as an equation for φ . The assumption on the spatial variation of $u_{1,2}$, along with a fixed boundary condition on the base of the bar and the fact that $u_{1,3}$ has to vanish, implies that $u_{1,2} \equiv g$ be a function of time alone, so that the term $T(x, t) \equiv \tau(g(t) - \varphi(x, t))$ in (38) does not pose a problem. However, the term $(\chi_R)_{12}$ is problematic as it cannot be written as a function of φ . For the sake of simplicity in this special problem, *we will make the approximation that it is simply a function of φ denoted by P* . Thus the governing equations we consider are

$$\boxed{\begin{aligned} \varphi_t &= \frac{(\varphi_x)^2}{\tilde{B}(|\varphi_x|)} [\tau(g(t) - \varphi) + \varepsilon \varphi_{xx} + P(\varphi)] \quad \text{hard loading} \\ \varphi_t &= \frac{(\varphi_x)^2}{\tilde{B}(|\varphi_x|)} [\tau(x, t) + \varepsilon \varphi_{xx} + P(\varphi)] \quad \text{soft loading.} \end{aligned}} \quad (39)$$

Equation (39) governs the evolution of (generally incompatible) plastic shear strain in the bar; spatial gradients of the profile represent the dislocation density field ((36)-(37)) with individual discrete dislocations (more precisely, dislocation walls) represented by a sharply localized φ_x field or, alternatively, a sharp transition front in the φ field.

Under hard loading (displacement control), $g(t)$ represents the average applied engineering shear strain on the bar, that, under the controlling assumptions, can only vary at most with time. Under soft loading (traction control), $\tau(x, t)$ represents the applied shear stress on the top surface of the bar (of course, keeping in mind that constraints would have to be in place that can provide the required reaction tractions on the lateral surface of the cylinder; admittedly, this is not a practically realistic requirement).

The function $g(t)$ is defined as follows: by assumption, let $u_{1,2} = g_0(x_3, t)$ where g_0 is any function of the arguments shown. Then, $u_1(x_1, x_2, x_3, t) = g_0(x_3, t)x_2 + h(x_1, x_3, t)$, where h is another function of the arguments shown. We now assume that the base of the bar is at $x_2 = 0$ and is held fixed, i.e. $u_1(x_1, 0, x_3, t) = 0 \Rightarrow h = 0$. The applied displacement at the top of the cylinder, $x_2 = l$, is given as $g_0(x_3, t)l$; but we need, by assumption, that $u_{1,3} \equiv 0$. Then $g_0(x_3, t) = g(t)$, where g has the physical meaning mentioned in the last paragraph.

As for boundary conditions, we either consider the Cauchy problem on the domain $(-\infty, \infty)$, or with Nuemann conditions $\varphi_x = 0$ at both ends of a finite bar.

We note that this problem has been intentionally set up to be simple enough so that force equilibrium is trivially satisfied and hence does not play a role in the plastic strain evolution, the latter being directly controlled by the applied boundary conditions. In fact, stress fields arising from any solution (39) is a genuine static solutions of balance of linear momentum without any approximation on inertia.

4.1 $P(\varphi)=0$, hard loading; exact solutions for equilibria in a special case and formulation of questions of stability

We deal with (39)₁ under the assumption that g is an arbitrarily fixed constant, i.e. the time dependence of the loading is not considered.

The equation is

$$\varphi_t = \frac{F(\varphi_x)}{B} [\varepsilon \varphi_{xx} + \tau(g - \varphi)], \quad (40)$$

where, from (27)₂ candidates for F are

$$\begin{aligned} F(a) &= a^2 \quad \text{or} \\ F(a) &= |a| \end{aligned} \quad (41)$$

and we abuse notation and refer to both B, B^* as B .

We define the function τ as follows: let $\hat{\tau}$ be the following ‘periodic-cubic’ function:

$$\hat{\tau}(y) = -\frac{\mu}{2\left(\frac{\bar{\varphi}}{2}\right)^2} y \left[y^2 - \left(\frac{\bar{\varphi}}{2}\right)^2 \right] \text{ extended periodically beyond } \left[-\frac{\bar{\varphi}}{2}, \frac{\bar{\varphi}}{2} \right], \quad \mu > 0. \quad (42)$$

Because of natural physical considerations, we need

$$\tau(0) = 0 \quad ; \quad \mu = \tau'(0) > 0 \quad (43)$$

i.e. shear stress at no elastic strain should vanish and the elastic modulus at zero strain should be positive. Now define τ in (40) as

$$\tau(\gamma_e) = -\hat{\tau}\left(\gamma_e - \frac{\bar{\varphi}}{2}\right). \quad (44)$$

Question 0: Are there spatially varying, ‘dislocation like’ equilibria of the equation (e.g. $\tanh(x)$ type) for special values of g (or a family of spatially inhomogeneous equilibria parametrized by g)? Of course, there is a 1 parameter family of spatially homogeneous equilibria.

Inhomogeneous equilibria: It can be checked that the one-parameter family of profiles

$$\varphi_{eq}(x; g) = g - \frac{\bar{\varphi}}{2} \pm \frac{\bar{\varphi}}{2} \tanh\left(\sqrt{\frac{\mu}{4\varepsilon}} x\right) \quad (45)$$

are equilibria. To see this, define $\gamma_e := g - \bar{\varphi}$ and note that $\gamma_e(x) - \bar{\varphi}/2$ corresponding to the profiles in (45) belong to the range $[-\bar{\varphi}/2, \bar{\varphi}/2]$. Next note that the periodic-cubic defined in (42) agrees with the actual cubic function of the same form on the interval $[-\bar{\varphi}/2, \bar{\varphi}/2]$. Let us call this ‘actual’ cubic, i.e. without periodic extension as in (42), $c(\cdot)$. Now for $0 \leq \gamma_e(x) \leq \bar{\varphi}$, which is the range of values covered by the elastic strain γ_e of the profiles in (45), a calculation for the profiles (45) shows that $\varepsilon(\varphi_{eq})_{xx}(x) = c(\gamma_e(x) - \bar{\varphi}/2)$, for each x in $(-\infty, \infty)$. But for $0 \leq \gamma_e \leq \bar{\varphi}$, $c(\gamma_e - \bar{\varphi}/2) = \hat{\tau}(\gamma_e - \bar{\varphi}/2) = -\tau(\gamma_e)$ by construction of c and $\hat{\tau}$ and (44), which implies $\varepsilon(\varphi_{eq})_{xx}(x) + \tau(\gamma_e(x)) = 0$ for all x in $(-\infty, \infty)$ for the profiles (45). Of course, by design, τ satisfies the physical requirement (43). The problem definition and special solution have been achieved by inspection: we consider admissibility of equilibria of the physically desired form, i.e. $A + B \tanh(sx)$, (A, B, s constants), and pick the constants and design the function τ to satisfy physical requirements and equilibrium.

Now consider the equilibrium for $g = g_*$. Consider the PDE with $g(x, t) = g_* + \delta, \delta > 0$, where g_*, δ are constants, and initial condition

$$\varphi(x, 0) = \varphi_{eq}(x; g^*). \quad (46)$$

Question 1: The question is whether there exist travelling wave solutions (with non-zero velocity, and hopefully ‘dislocation-like’) for equation (40) with constant $g = g_* + \delta$ and if the initial condition (46) is attracted to such a travelling wave as $t \rightarrow \infty$ or to other equilibria that exist, in particular $\varphi_{eq}(x; g^* + \delta)$. For $g_* = 0$ if such a travelling wave exists for some $\delta_p > 0$ to which $\varphi_{eq}(x; 0)$ is attracted, then we would have shown the existence of a ‘Peierls strain’ in the model.

Traveling waves: We call a function of the form $\theta(x, t) := f(x - ct)$, c a constant, a travelling wave solution to (40) if it satisfies it with $c \neq 0$. Here f is a function of a single variable. On considering the governing equation of a traveling wave solution

$$-f'c = \frac{F(f')}{B} \{ \varepsilon f'' + \tau(g_* + \delta - f) \} \quad (47)$$

it can be checked that $\varphi_{eq}(x - ct; g^*)$ is not a travelling wave solution to (40) with $g = g^* + \delta$, for $\delta \neq 0, |\delta| \ll 1$. In this sense, it may be said that the model has a Peierls barrier, in that these ‘dislocation’-like equilibria cannot be rigidly translated by changing the load. Question 1 above addresses the question of whether there exists load levels corresponding to which there are profiles that move rigidly and whether, upon additional loading, the equilibrium profiles displayed above in (45) can be deformed into ones close to these travelling waves.

Question 2: $\varphi_*(x, t) \equiv 0$ is an equilibrium solution. Is there a value of $g > 0$ in (40), say g_N , and further conditions (e.g. boundary conditions) for which φ_* becomes ‘unstable’ and some initial condition $\varphi_*(x) + \delta\varphi(x)$ (small perturbation) is attracted to the equilibria $\varphi_{eq}(x; g_N)$? If so, then we would have shown the possibility of nucleation within the model as a question of

dynamic instability (cf. Dayal and Bhattacharya (2006) in the context of peridynamic theory). The analogous question for g time-dependent can be similarly formulated.

As an interesting aside, it is important to realize that a time-parametrized family of equilibria defined by

$$\varphi_{eq}(x, t) = g(t) - \frac{\bar{\varphi}}{2} \pm \frac{\bar{\varphi}}{2} \tanh\left(\sqrt{\frac{\mu}{4\varepsilon}} x\right), \quad (48)$$

where $g(\cdot)$ is any non-constant, time-dependent loading program, is *not* a solution to the governing equation, for the same time-dependent loading, given by

$$\varphi_t = \frac{F(\varphi_x)}{B} \left[\varepsilon \varphi_{xx} + \tau(g(t) - \varphi) \right]. \quad (49)$$

Such are the curiosities of ‘quasi-static solutions’ of evolution equations, that may only be justified in an asymptotic sense corresponding to loading histories representing short bursts of rapid loading interspersed with long periods of loads held constant.

4.2 $P(\varphi) \neq 0$; equilibria for hard and soft loading in a special case

Recall that $P(\varphi)$ is a crude simplification for a term that is in reality a component of the non-local, *curl* projection of $\mathbf{R} = s(|\alpha|l) \partial G / \partial \chi$. At any rate, this needs constitutive specification. Let us make the assumption that

$$P(\varphi) := -2\tau(\hat{g} - \varphi), \quad (50)$$

where \hat{g} is a material-specific strain value. For analytical progress, let us assume the stress response in this case to be given by

$$\tau(\gamma^e) = \hat{\tau}(\gamma^e) \quad (51)$$

where $\hat{\tau}$ is defined by (42).

Equilibria, hard loading: For the case of hard loading, the governing equation for the plastic strain evolution becomes

$$\varphi_t = \frac{F(\varphi_x)}{B} \left[\varepsilon \varphi_{xx} + \hat{\tau}(g - \varphi) - 2\hat{\tau}(\hat{g} - \varphi) \right], \quad (52)$$

where F is defined in (41). As before, we consider the simpler problem of (52) with a constant, but arbitrary, value of the load.

It is clear that spatially homogeneous profiles are equilibria, regardless of the value of the applied strain g . Spatially inhomogeneous equilibria can be written down for (52), stated for the special value of $g = \hat{g}$, as

$$\hat{g} \pm \frac{\bar{\varphi}}{2} \tanh\left(\sqrt{\frac{\mu}{4\varepsilon}} x\right). \quad (53)$$

It is easy to check that the functions in (53) cannot serve as travelling wave profiles for (52) stated for $g = \hat{g} + \delta, \delta \neq 0, |\delta| \ll 1$.

Question 3: A natural question that arises is the following one related to nucleation: for (52) stated for $g = \hat{g}$ or for g time-dependent, does the homogeneous solution $\varphi(x, t) \equiv 0$ lose

stability so that a minor perturbation on $\varphi(x, t) \equiv 0$ as initial condition drives the solution of (52) to the profiles given in (53)?

Equilibria, soft loading: For soft loading, we consider the governing equation

$$\varphi_t = \frac{F(\varphi_x)}{B} [\tau(x) + \varepsilon \varphi_{xx} - 2\hat{\tau}(\hat{g} - \varphi)], \quad (54)$$

where $\tau(x)$ is the applied traction on the top surface of the bar.

Again, spatially homogeneous profiles are equilibria, regardless of the nature of τ . For $\tau(x) \equiv 0$, it is easy to check that

$$\varphi_{eq}^s(x) := \hat{g} \pm \frac{\bar{\varphi}}{2} \tanh\left(\sqrt{\frac{\mu}{2\varepsilon}} x\right) \quad (55)$$

are equilibria of (54). For the case of $F(a) = |a|$, it is interesting that $\varphi_{eq}^s(x - ct)$ is a travelling wave solution to (54) stated for τ a non-zero constant. Noting that (55) represents spatially monotone profiles, i.e. the sign of the first derivative is either positive or negative at all x , the constant speed of the travelling wave is given by

$$c = -\text{sgn}\left(\left(\varphi_{eq}^s\right)_x\right) \frac{\tau}{B}. \quad (56)$$

Thus, this case corresponds to the classical conclusion of Peierls (1940) of a continuum theory not having a Peierls barrier. However, as is clear from our model and analysis, translational invariance of the theory is not a sufficient condition for the absence of a Peierls barrier in this dynamical point of view.

Dynamical stability questions analogous to the $P(\varphi) = 0$ case can also be formulated in these cases for $P(\varphi) \neq 0$.

5. Implications for Meso/Macroscopic Plasticity

The question we now address is what information can be inferred about the evolution of plastic distortion averaged over space and/or time, given the microscopic evolution equation (29). From (28)-(29) we note that the plastic distortion evolution may be written in the form

$$\dot{\mathbf{U}}^P = \frac{1}{\tilde{B}(|\boldsymbol{\alpha}|)} \boldsymbol{\alpha} \times \mathbf{X}(\mathbf{S}\boldsymbol{\alpha}), \quad (57)$$

where \mathbf{S} is an appropriate second-order tensor. Now,

$$\boldsymbol{\alpha} \times \mathbf{X}(\mathbf{S}\boldsymbol{\alpha}) = (\boldsymbol{\alpha}\boldsymbol{\alpha}^T) \mathbf{S}^T - \boldsymbol{\alpha} \mathbf{S} \boldsymbol{\alpha}. \quad (58)$$

We assume that on solving the microscopic theory and probing the dislocation density field around any point \mathbf{x} , the $\boldsymbol{\alpha}$ can be expressed in the form

$$\begin{aligned} \boldsymbol{\alpha}(\mathbf{x}, t) &= |\boldsymbol{\alpha}(\mathbf{x}, t)| d(\mathbf{x}, t) \mathbf{D}(\mathbf{x}, t) \\ \mathbf{D}(\mathbf{x}, t) &:= \sum_{l=1}^{N(\mathbf{x}, t)} \mathbf{m}^l(\mathbf{x}, t) \otimes \mathbf{l}^l(\mathbf{x}, t), \quad d = \begin{cases} 1/|\mathbf{D}| & \text{if } \mathbf{D} \neq \mathbf{0} \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (59)$$

where d is an $O(1)$ non-dimensional numerical factor, $N(\mathbf{x}, t)$ is an integer that represents the number of dislocation segments involved in a possible junction at the location (\mathbf{x}, t) , $\mathbf{m}^l(\mathbf{x}, t)$ is

a unit vector representing the Burgers vector of the I^{th} dislocation segment that may be involved in the junction, and similarly $\mathbf{l}^I(\mathbf{x}, t)$ is the line direction of the same segment. Then

$$\begin{aligned} [(\boldsymbol{\alpha}\boldsymbol{\alpha}^T)\mathbf{S}^T]_{ir} &= |\boldsymbol{\alpha}|^2 d^2 D_{ip} D_{kp} \delta_{jr} S_{kj}^T \\ [\boldsymbol{\alpha}\mathbf{S}\boldsymbol{\alpha}]_{ir} &= |\boldsymbol{\alpha}|^2 d^2 D_{ij} D_{kr} S_{kj}^T \\ \mathbf{S} &= \mathbf{T} + [-\varepsilon \operatorname{div} \operatorname{grad} \boldsymbol{\chi} + \boldsymbol{\chi}_R]^T, \end{aligned} \quad (60)$$

and defining fourth-order structure tensor fields

$$\begin{aligned} [\mathbb{Z}^1(\mathbf{x}, t)]_{irkj} &= D_{ip}(\mathbf{x}, t) D_{kp}(\mathbf{x}, t) \delta_{jr} \\ [\mathbb{Z}^2(\mathbf{x}, t)]_{irkj} &= D_{ij}(\mathbf{x}, t) D_{kr}(\mathbf{x}, t), \end{aligned} \quad (61)$$

the evolution of (asymmetric) plastic distortion takes the form

$$\dot{\mathbf{U}}^p = \frac{|\boldsymbol{\alpha}|^2}{\tilde{B}(|\boldsymbol{\alpha}|)} d^2 [\mathbb{Z}^1 - \mathbb{Z}^2] : (\mathbf{T} - \varepsilon \operatorname{div} \operatorname{grad} \boldsymbol{\chi} + \boldsymbol{\chi}_R). \quad (62)$$

To define spatially averaged behavior, we resort to the use of ‘filters.’ For a microscopic field f given as a function of space, we define the meso/macroscopic space averaged field \bar{f} as follows:

$$\bar{f}(\mathbf{x}, t) := \frac{1}{\int_{\Omega(\mathbf{x})} w(\mathbf{x} - \mathbf{x}') d\mathbf{x}'} \int_B w(\mathbf{x} - \mathbf{x}') f(\mathbf{x}', t) d\mathbf{x}', \quad (63)$$

where B is the body. In the above, $\Omega(\mathbf{x})$ is a bounded region within the body around the point \mathbf{x} with linear dimension of the order of the spatial resolution of the macroscopic model we seek. The averaged field \bar{f} is simply a weighted, running space-average of the microscopic field f over regions whose scale is determined by the scale of spatial resolution of the averaged model one seeks. The weighting function w is non-dimensional, assumed to be smooth in the variables \mathbf{x}, \mathbf{x}' and, for fixed \mathbf{x} , have support (i.e. to be non-zero) only in $\Omega(\mathbf{x})$ when viewed as a function of (\mathbf{x}') . Applying this operator to (62) (now phrased in terms \mathbf{x}'), we obtain

$$\frac{d}{dt} \bar{\mathbf{U}}^p = \dot{\bar{\mathbf{U}}}^p = \bar{\varpi} \overline{d^2 [\mathbb{Z}^1 - \mathbb{Z}^2] : (\mathbf{T} - \varepsilon \operatorname{div} \operatorname{grad} \boldsymbol{\chi} + \boldsymbol{\chi}_R)} \quad (64)$$

under the assumption that

$$\varpi \approx \bar{\varpi} \quad (65)$$

where

$$\varpi = \frac{|\boldsymbol{\alpha}|^2}{\tilde{B}(|\boldsymbol{\alpha}|)}. \quad (66)$$

The assumption (65) is valid when there is a large number of dislocation segments within the averaging volume. It is also assumed that the average magnitude of $\boldsymbol{\alpha}$ within a dislocation core is the same at all locations where a dislocation segment is present.

The physical dimensions of \tilde{B} is given by $[\tilde{B}] = [\mathbf{T}][\boldsymbol{\alpha}]/[\mathbf{V}]$. Let the average stress magnitude in the core of a single dislocation be $\sim \sigma^*$. The average magnitude of the dislocation density in

the core is $\sim b/b^2$. According to Nabarro (1987, p. 506-507) the free-flight velocity from experiment for a single dislocation is $v_{\text{exp}} = 1\text{m/s} \sim 100\text{m/s}$. Thus, the magnitude of \tilde{B} is $\sim \sigma^*/bv_{\text{exp}}$ and the magnitude of $\bar{\omega}$ is $\sim v_{\text{exp}}/b\sigma^*$. Let t^* be the time-resolution of observations and define $s = t/t^*$. Then (64) may be rewritten as

$$\frac{d}{ds}\bar{U}^p = t^*\bar{\omega}f\sigma^* \left\{ \frac{1}{f\sigma^*} d^2[\mathbb{Z}^1 - \mathbb{Z}^2] : (\mathbf{T} - \varepsilon \text{div grad } \boldsymbol{\chi} + \boldsymbol{\chi}_R) \right\} \quad (67)$$

where f is some non-dimensional constant. Let us define the nondimensional viscosity, ν , by

$$\frac{1}{\nu} := t^*\bar{\omega}f\sigma^*. \quad (68)$$

Assuming the magnitude of t^* and b to be $1\text{s} \sim 10^{-3}\text{s}$ and 10^{-10}m , respectively, and $f = 10^{-3} \sim 1$, we have

$$\frac{10^{-3} \cdot 1 \cdot 10^{-3}}{10^{-10}} \leq \frac{1}{\nu} \leq \frac{1 \cdot 10^2 \cdot 1}{10^{-10}}; \quad (69)$$

Hence, the viscosity $\nu \ll 1$, and (67) takes on the form of a singularly perturbed system. Equation (67) implies that on occasions when the magnitude of the spatially averaged plastic distortion rate on the t^* time-scale is not too large, say $O(1/t^*)$, i.e. at most $\sim 1/t^*$, the constraint

$$\mathcal{R} := d^2[\mathbb{Z}^1 - \mathbb{Z}^2] : (\mathbf{T} - \varepsilon \text{div grad } \boldsymbol{\chi} + \boldsymbol{\chi}_R) \approx \mathbf{0}, \quad (70)$$

has to be satisfied, and it may be thought of as a tensorial yield criterion governing *rate-insensitive* plastic response at the macroscopic scale. It is worthy of note that our consideration does not state that the constraint (70) has to hold at all times; indeed it allows for high-rate deformations where the yield condition can be seriously violated. It seems to be certainly within the realm of possibility that \bar{U}^p evolution on the t^* time-scale corresponding to variations in applied boundary loads shows two different regimes; one very slow to vanishing, and the other an order(s) of magnitude more rapid, but nevertheless both regimes being at most $\sim 1/t^*$. Were this to be the case, macroscopic yielding from elastic response would have been predicted, providing a fundamental basis for qualitative features of phenomenological, macroscopic, rate-independent plasticity theory. Such studies, along with the prediction of episodes of onset and arrest of fully rate-sensitive response with significant deviations from the yield set would be practically useful results⁴; however, they clearly require a deep understanding of the stability properties of the yield set viewed as a ‘limit set’ of trajectories of the dynamics (67) with all external influences held constant. For a glimpse of what is possible in situations that can only be considered ‘simple’ in the context of our general theory see, e.g. Carr and Pego (1989) and, in the context of ODE theory, Artstein and Vigodner (1996), Artstein (2002) (the latter has low-dimensional illustrative examples of coupled slow-fast motions with non-trivial limit motions).

Since evolution via (67) is naturally viewed in the t^* time-scale, the condition (70) may be viewed as valid continuously over periods of the order of t^* ; consequently, (70) may also be viewed as valid when averaged over a period of t^* . Assuming the incompatible slip energy G

⁴ Preliminary numerical computations indicate that both yielding type response and intermittency are within the predictive scope of the model, at least in the 1-d case.

can be characterized from atomistic/quantum studies, characterization of the time-averaged form of (70) from theoretical homogenization or lattice-statics calculations or simulations of the microscopic theory described in section 3 seems to be a worthy and practically useful challenge in defining macroscopic plastic response. When replacing pointwise-field values at (\mathbf{x}', t') of the individual terms appearing in (70) by their space-time averages over $\Omega(\mathbf{x})$ and time interval t^* around the instant t may be justified, (70) takes the instructive form (with space-time averages now denoted by overhead bars),

$$\left[\overline{\mathbb{Z}^1} - \overline{\mathbb{Z}^2}\right] : \left[\overline{\mathbf{T}} - \varepsilon \operatorname{div} \operatorname{grad} \overline{\boldsymbol{\chi}} + \overline{\boldsymbol{\chi}_R}\right] = \mathbf{0}. \quad (71)$$

The form (71) begins to suggest possible physical origins of the terms commonly used in phenomenological plasticity for work-hardening, the “gradient effects” of Aifantis (1984, 1987)⁵, and plastic anisotropy and spin. From this point of view, it is interesting to note the nonlocality inherent in work-hardening response. Curiously, if one were for the moment to assume the leading structure tensor term in (71) to be the fourth-order identity, then the skew symmetric part of the equation poses an interesting integro-differential constraint on the skew part of $\boldsymbol{\chi}$.

We note here that the association of high gradients of slip in a core along with the presence of many cores as the primary cause for rate-insensitive macroscopic response is different and complementary to other mechanisms for the phenomena based on pinning due to postulated rugged energy landscapes (Puglisi and Truskinovsky, 2005) or extrinsic obstacles (e.g. Bhattacharya (1999), in the context of phase boundary pinning). It is also interesting to note that the assumption of a high dislocation content within the averaging volume leads to wave-like response completely dropping out of macroscopic response (when the average plastic distortion rate is small). At the mesoscopic scale, this key assumption of a uniformly high dislocation density in space cannot be made; then, the transport terms remain, but the microscopic theory is practically untenable. What the form of the governing equations should be at this scale is a key challenge for rigorous mechanics and mathematics. Some promising heuristic advances coupled with numerical work have been made recently (Acharya and Roy, 2006; Roy and Acharya, 2006; Taupin et al., 2007; Acharya et al. 2008; Taupin et al., 2008; Fressengeas et al., 2009).

6. Comparison with the structure of phase-field models and level set evolution

We end with a couple of remarks on the structure of our theory. While the manner in which the constitutive structure (27) is defined, along with the assumption (13) and the use of a conservation law, i.e. (10), may be reminiscent of (time-dependent) Ginzburg-Landau, local-energy-minima seeking phase-field type models or Cahn-Hilliard models, the dynamics implied by our theory is different from that implied by these formalisms. Roughly speaking, this is because our situation corresponds to having a conservation law for the gradient of the order parameter (plastic distortion) based in the kinematics of convective transport, along with a ‘surface energy’ term – alternatively, if one considers the dislocation density as the order parameter, then there is a conservation law but no surface energy. To see one of these comparisons in the simplest possible context, consider an energy of the form

⁵ Although beyond the Laplacian and the sign in front of it, the details are quite different. Note that, roughly, $\boldsymbol{\chi}$ corresponds to $-\mathbf{U}^p$.

$$\psi = \hat{\psi}(g - \varphi) + \frac{1}{2}(\varphi_x)^2, \quad (72)$$

where g is a constant. Then the corresponding Ginzburg-Landau model would be

$$\begin{aligned} \dot{\varphi} &= -\Gamma \frac{\delta\psi}{\delta\varphi} \quad \Gamma = \text{mobility} \\ \Rightarrow \dot{\varphi} &= \Gamma(\varphi_{xx} + \tau(g - \varphi)), \end{aligned} \quad (73)$$

and it is instructive to compare this with (40). Of course the all important difference is the $F(\varphi_x)$ term in our dynamical model, one of the major effects of which is in providing the singular perturbation structure in the averaged macroscopic model of plasticity mentioned in Section 5. This comment is also the only relevant one we are able to make in a comparison to the static, energy minimizing, phase field framework of Koslowski et al. (2002), where it is not clear exactly what *physical* criteria is used to pick amongst multiple local minima. Also, it is well-known that the Cahn-Hilliard formalism yields fourth-order equations whereas ours is simply second order.

Finally, we mention that our equation (39) (with $\tilde{B} = B|\varphi_x|$) in *the scalar case* may be interpreted as the evolution of a level-set with velocity given by the Ginzburg-Landau driving force. Thus it is natural to expect transfer of qualitative properties like pinning, or lack thereof, between our model and level-set propagation of this specific type.

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